Good moling ... oh, good morning!

There are MOLARIFIC opportunities at DARPA within the Defense Science Office and Microsystems Technology Office. Today, we will talk about a program to bring electronics into the penultimate Lilliputian regime using self- assembled molecules.

This is a program we call "Moletronics" or Molecular Electronics.

We call it Moletronics cause we are using molecules or molecular scale components for computation.

The DARPA Moletronics program intends to demonstrate the development of a new computational technology that will make the electronics age of today look like a rowboat as compared to a nuclear submarine.

To create discovery beyond silicon, the DARPA Moletronics program will chemically assemble systems with insanely high device densities (scaleable to 1012 device/cm2) that are amenable to greatly simplified manufacturing fabrication.

To put things in perspective, today's microprocessors have about 108 devices/cm2-- 1012 devices/cm2 is big time dense.

Molecular Electronics is defined as a technology based on using molecular scale components such as single molecules, carbon nanotubes, nano-wires, etc. that function as electronic components.

Using these molecular-scale components, one can see that the size benefits of Moletronics are incredible.

Here we show that when standard p-n rectifying diodes, ones that you could buy at Radio Shack, are replaced with single molecules, the areal size benefit is 10,000x. Experimentally it has been demonstrated that single molecules do exhibit rectifying behavior by a number of groups.

This is NOT science fiction.

Here we show the information content of various media from color photos, to the human brain to annual television. The byte content from my presentation isn't up there because it is embarrassingly low.

Anyhow, adding these up, the total sum of information in humanity is around 10^20 bytes. Just imagine if we had a mole of bytes.

A mole is 6 x 10^23 devices in this context.

The concept of a mole of information is mind-boggling. Stretching our imaginations into the future, you could literally hold all the information in human history in the palm of your hand!

One driver for Moletronics is that Si technology will hit a technological brick wall in the not-too-distant future. One of the greatest technological issues regarding Si CMOS is how to obtain nanoscale features in a high-throughput and inexpensive fashion.

Having said this, it has been predicted that we will hit the Si technological brick wall for years, but the daggon wall keeps on moving.

There is one wall that doesn't move in the right direction. This wall is often called Moore's second law, which shows that the cost of Si fab lines grows exponentially with time. Moore's first law deals with the exponential decrease in device feature size with time.

The graph above plots Moore's first law against Moore's second law.

One can see that unless we change the way things are done, i.e., conventional fab facilities using lithography, by the time we reach molecular scale sizes the cost of fab lines will be 10 trillion dollars (about 1000x DARPA's annual budget!)

One of the objectives of Moletronics is to literally knock this economic wall down using hierarchical self-assembly processes. I will talk more about this in a moment. More specifically, we hope to knock the Si Goliath wall down by literally throwing molecules, nanotubes, and nanowires at it! This is a wall that even Ronald Reagan couldn't knock down.

To accomplish the Moletronics goal, there are three parallel tasks.

The first task is the development and optimization of molecular devices such as switches, multistate molecules, and molecules exhibiting highly non-linear characteristics.

The second task is learning how to build a Moletronic computer made from these molecular devices. We believe they will be manufactured by hierarchical self- assembly processes. Hierarchical self-assembly is a set of processes that will first assemble individual devices, then create functional circuits or blocks from those devices, and finally put together the ensemble from the blocks. It is a bottom-up manufacturing process whereas current microelectronics fabrication is based on top-down manufacturing using lithography.

The third task is the development of circuit architectures. These architectures encompass how to program the molecular circuit as well as exhibit defect tolerance. Moletronic circuits will have defects. We will have to cope with them, in the vernacular, the fleas come with the dog. Approaches to quantify the level of defects that can be tolerated, the time needed to find and route around the defects, and the time to program a circuit with large numbers of devices need to be developed under the architecture umbrella. Let me discuss in greater lengths these three essential tasks.... The first task is molecular devices. We need to understand how to chemically design a desired electronic property into a molecule, whether the molecule is used for logic, memory, or gain.

As one example, work at Yale and Rice University has demonstrated the ability to chemically design-in electronic properties into their memory molecules. They literally "dial in" the performance attributes of their memory molecules by synthesizing different side groups (nitro or amine groups).

For this work, the molecular memories are a monolayer of molecules sandwiched between two crossing Au electrodes.

It is the reduction/ oxidation of the molecule that determines whether it is conducting (bit "1") or insulating (bit "0").

Here we show a different molecular device from UCLA and HP Labs.

Logic gates were fabricated using several switches. The makeup of the switches is pretty simple: a monolayer of redox-active rotaxane-based molecules are sandwiched between metal electrodes, much like a slab of meat between two slices of bread. Several switches were configured together to produce AND and OR logic gates. The truth table of an "AND" gate is such that a high response is only recorded when the inputs are all high. As you can see in the graph, incredibly respectable "AND" gates have been made with molecules.

Using molecular scale components in a crossbar fashion, the Mountains of Silicon will soon become the Molehills of Moletronics.

Here we show the difference in size between Moletronic crossbar logic and that obtained with conventional silicon.

By crossbar we just mean that 2 wires cross each other and in between the wires is a mono-layer of molecules.

Crossing the chasm from the nano-world to the micro-world is a grand challenge of Moletronics, in fact it is for any nanoscience program.

Our specific challenge is how to get input/output to the outside world, that is, how to plug a beaker of molecules into an electrical outlet.

We envisage this to occur in part by using a hierarchical ordering of several self-assembly steps.

Self-assembly is a process whereby molecular components naturally (spontaneously) assemble into a desired pattern. It is not a pick and place, nor a slice and dice technology. Patterns naturally form under the guiding arm of thermodynamics, or better described as the lowest energy configuration. Costly lithography is not required in self-assembly processes.

Here we show a simple cartoon of a self-assembly process in which chemical bonding is used to hoard an array of molecules on a substrate.

Next we show how self-assembly can be used to form aligned wires.

The wires in this case are only 10 atoms wide, 2 atoms high and microns long. The process is unbelievably simple, but incredibly revolutionary.

To make the wires all that's required is to deposit a sublayer of Er on the Si wafer and then anneal it around 700C.

Upon annealing the Er film, $ErSi_2$ nucleates and takes off in one direction, but not the other. Thus, the question, why should it go only in one direction? The reason is due to anisotropic lattice mismatch.

The structure of ErSi2 is relatively lattice matched in the <110> direction, but mismatched by over 6% in the other of the (001) plane of Silicon.

The thermodynamics is driven, that is the energy is minimized, when growth occurs along the lattice matched direction.

The aligned wires are 1/2 of our cross-bar architecture.

The second half of the cross-bar architecture can be assembled using water -- yes water. Researchers at Penn State have shown that hydrophobic/ hydrophilic interactions (water hating/water loving) can be used to precisely assemble a cross- bar pattern. Just like the last process, this one is simple too.

Take 2 glass wafers.

Deposit a few Au patterns on the glass; the glass is water loving; the Au patterns contain water hating thiol molecules.

Upon joining the glass wafers together, the Au patterns precisely align with each other.

Precise alignment occurs because the hydrophobic ends and the hydrophilic ends meet each other, respectively to achieve the lowest surface energy.

Another beautiful example of how amazing things happen in love/hate relationships!

Again, all of this alignment was done without pick and place equipment, nor lithography!

The last two examples show how to make aligned wires, and then how to precisely cross these wires using two different self-assembly processes.

The two processes are hierarchical in nature. Hierarchy is a royal ordering of processing steps.

The hierarchy starts with lower-order steps (molecules to form a nano-block).

An example of a nano-block is a memory or logic element.

The next level of assembly is the connection of nano-blocks into an electronic module. Here a module is able perform both logic and memory, that is, it does a computation and stores the information.

The highest level of assembly involves hooking up the electronic modules to the outside world. This would create a molecular circuit or chip.

It is anticipated that hierarchical self-assembly will create a cost-effective manufacturing process.

The reason: we have replaced expensive lithographical processes with self-assembly processes.

Hierarchical self-assembly is a bottom-up manufacturing process.

In parallel with this assembly approach, Moletronics must also apply an architecturally driven, top-down route to layout the blueprint of the Moletronic circuits.

A paramount challenge of Moletronics is to demonstrate that the circuit architecture is scalable to 1011 devices and to densities equivalent to 1011/cm2. That is: how do you communicate with 1011 devices in a timely fashion?

Another unique feature of Moletronics circuits is that they will have defects; we are dealing with molecules and thermodynamics.

The parachute is analogous to today's Pentium - one defect (or rip) could kill 'ya. The fence analogy is more akin to Moletronics. There may be defects in the fence, but it will still largely function.

The bottom line is -- we've got defects and we've got to cope with them in our architectures.

Other architectural scalability issues include power dissipation, how long it will take to read and write the Moletronic circuit and how long it will take the test the circuit.

Here we provide two ways in which one could use Moletronic circuits.

For the first case, we could use molecular-scale components to create a supercomputer with 10^12 devices in 1 cm2 area.

The power dissipated would generate about 10,000 Watts, quite a bit of power to have on your lap. This illustrates that we have to think carefully about scaling.

The second example is one for nanocomputers that are at a density of 10^12 devices/cm^2. At this density, we could place a something with comparable power to a Pentium in an area of about 10^-- 3 cm2, literally a Pentium on a pin head! Perhaps this may be the best use of molecular computers for reasonable computational power in an extremely small, low-power package.

This opens up opportunities for nano-computers woven into fabrics or into paint on the walls.

Moletronics will require new ways to think about architecture and how to compile and program the molecular computer. For example, Moletronic circuits will be programmed after being built. In this sense, the molecular computer has to be "taken to school." This is in contrast to conventional Si, programming is done during fabrication through mask sets.

From the software side, defect search algorithms are extremely important.

With device densities of 1011/cm2, it can become a daunting task to find the defects quickly. It is imperative that sophisticated search algorithms be developed to determine how long it will take to find and subsequently route around defects.

It is a hard task, but we can stand on the shoulders of giants and learn a few tricks.

As one example, the defect search algorithms are analogous to web search engines in the Internet.

The web requires discovery to use it; this is accomplished using search engines. Moletronics will also require discovery to use it.

In this case, the discovery will be to program the circuit as well as finding the defects so that they can be by-passed.

Lots of advanced research is going on in the realm of web search engines, we plan exploiting it and hopefully improving upon it in Moletronics.

To conclude, Moletronics involves both a bottom up and a top down approach.

The bottom up approach is to exploit self-assembly schemes, and concoct new nanoscale materials and phenomena.

We hope that self-assembly brings about a new era in cost-effective manufacturing.

The top down approach is largely architecturally and algorithm driven. In this case, we must exploit architectures that are defect tolerant and ones that are scalable.

We will also require algorithm development to program the molecular computer and search for its defects.

If you have any ideas on algorithm or architecture development or general comments or even criticisms about Moletronics, Christie Marrian and I sure would like to hear them. We have an active BAA on the streets, please look it up and see what DARPA is after. We need your ideas and talents to make this happen.

Thank you. Remember ... Keep thinking MOLETRONICS.